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Experimental and theoretical study of the crystal-field levels and hyperfine and electron-phonon interactions in LiYF4:Er3+

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Abstract

We have measured high resolution absorption spectra for the 4I15/2→4I13/2, 4I11/2 infrared transitions of Er3+ ions in LiYF4. Positions of crystal-field levels and their widths were precisely determined and analyzed. Hyperfine structure of 167Er totaling ~0.2 cm-1 was observed. Experimental data are described by a theory that operates with a realistic model of the lattice dynamics and with the crystal-field parameters and electron-phonon coupling constants calculated in the framework of the exchange charge model. The hyperfine splittings of the odd mass number isotope 167Er are calculated taking into account both magnetic dipole and electric quadrupole hyperfine interactions. The simulated hyperfine structure is in good agreement with the experimentally observed one. The one-phonon relaxation rates within the 4I11/2 and 4I13/2 crystal-field manifolds are calculated using the correlation functions of the Er3+ ion and ligand displacements. The results of these calculations agree within an order of magnitude with the measured homogeneous linewidths of the corresponding zero-phonon transitions from the ground state at low temperatures.